10.1071/CH23061
Australian Journal of Chemistry

Supplementary Material

Exploring colorimetric detection of perfluorooctane sulfonate using micelle solubilised porphyrin

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Micelle Assembly Conditions

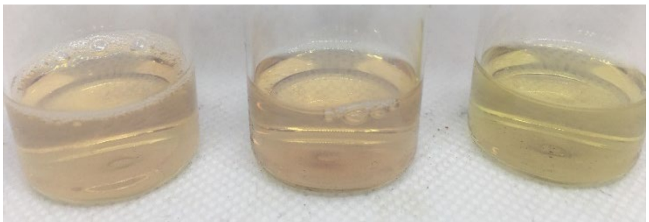

Fig. S1. Photograph of host **1** (1.8 x 10^{-5} M) in a TritonX-100 micelle solution (2.2 x 10^{-4} M) (left), and the colour difference observed with the addition of KPFOS (4.9 x 10^{-7} mol, 1 mL, final [KPFOS] 25 ppm) (middle), and PFOA (4.1 x 10^{-7} mol, 1 mL, final [KPFOS] 21 ppm) (right).

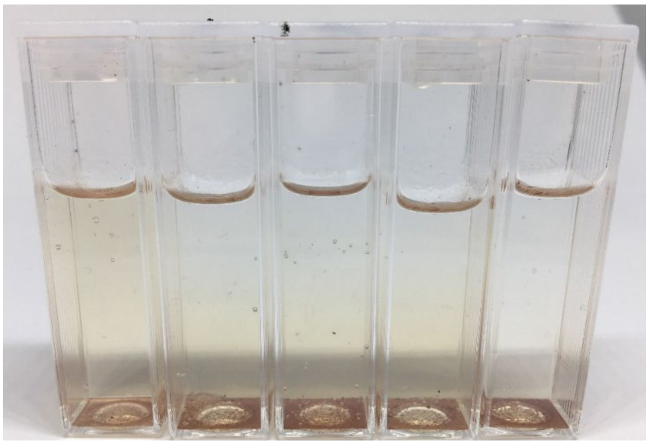

Fig. S2. Host **1** (4.5 x 10^{-5} M) in a CTAB micelle solution (1.8 x 10^{-3} M) assembled with dioxane as the dispersal solvent. From left to right there are increasing concentrations of KPFOS; 0, 0.7, 1.2, 1.7, and 2.3 ppm. Precipitation of host **1** is visible, increasing from left to right.

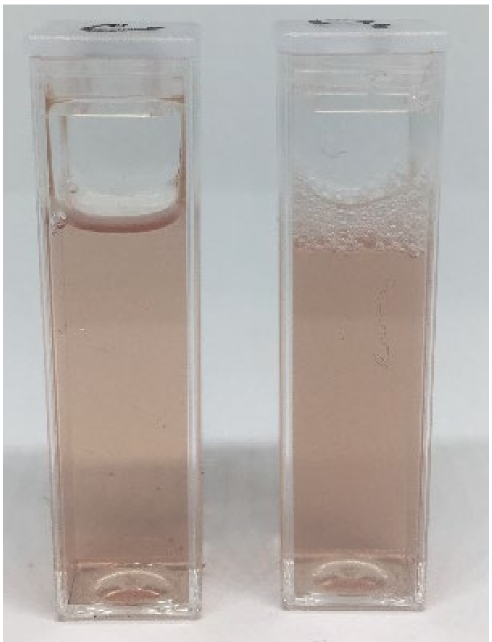

Fig. S3. Host **1** (4.7 x 10^{-5} M) in a Tergitol micelle solution (2.8 x 10^{-1} M) assembled with acetone as the dispersal solvent. There was no visible colour change detectable, but foaming was evident upon the addition of KPFOS (1.16 x 10^{-7} mol, 1 mL, final [KPFOS] 8 ppm) (right).

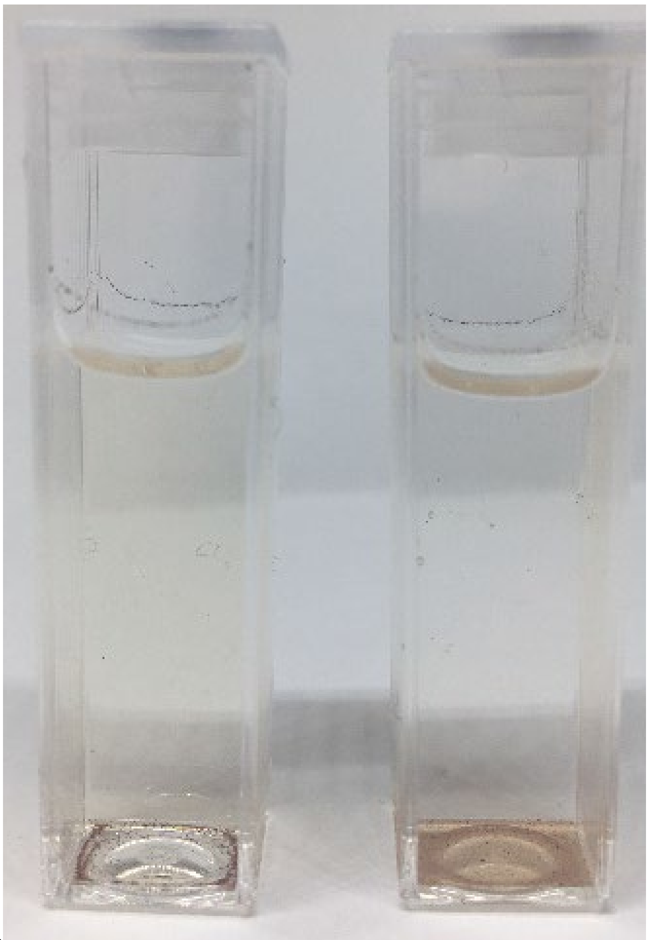

Fig. S4. Host **1** (1.8 x 10^{-6} M) in a SDS micelle solution (7.3 x 10^{-3} M) assembled with acetone as the dispersal solvent. Left shows the original colour, and rights shows the colour change and precipitation observed with the addition of KPFOS (9.8 x 10^{-9} mol, 0.5 mL, final [KPOS] 2.3 ppm).

Table S1. Comparison of absorption maxima for the Q-bands of porphyrin host **1** in micelle solutions and organic solvent.

		λmax [nm]	
Solution	**1** [mmol/L]	**Q IV (1,0)**	**Q III (0,0)**
1-CTAB micelle in THF:water	2.0 x 10^{-4}	520	595
1-CTAB micelle in DCM:water	2.0 x 10^{-4}	515	589
1-Triton^{TM}X-100 micelle in acetone:water	1.8 x 10^{-2}	520	591
1-SDS micelle in acetone:water	1.8 x 10^{-2}	523	595
1 in DCM	8.8 x 10^{-2}	515	589

UV-Visible Absorption Spectroscopy

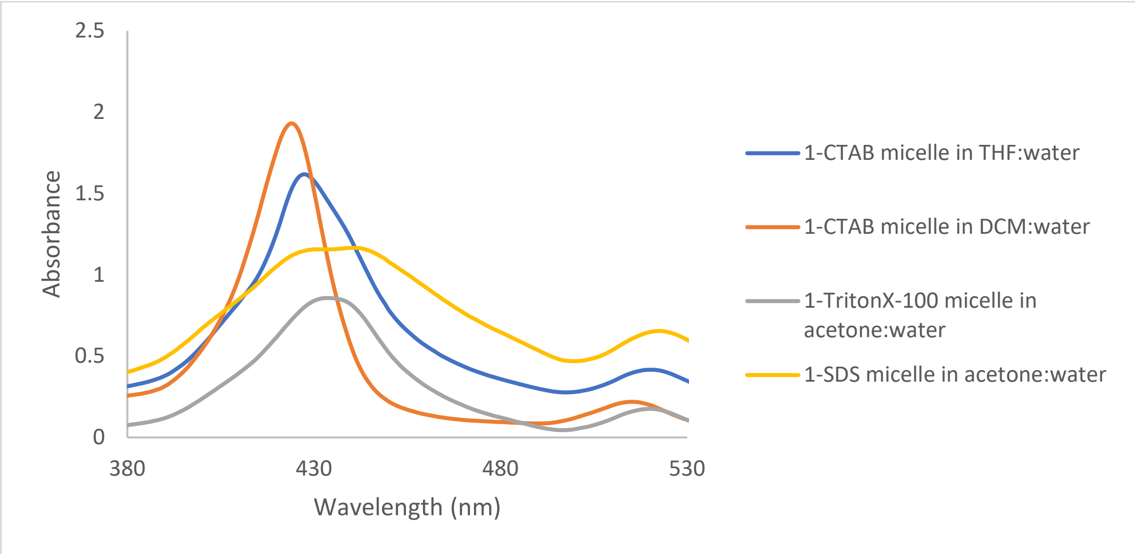

Fig. S5. UV-Visible absorption spectra showing the Soret band regions of host molecule **1** and different surfactants assembled in using a range of solvents.

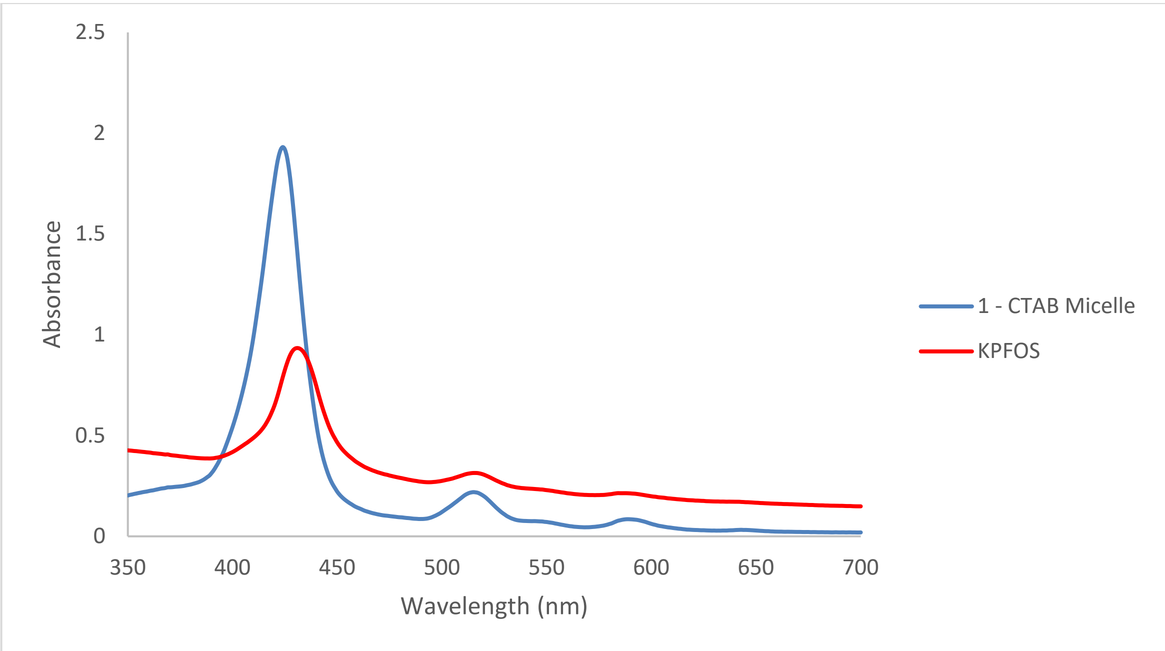

Fig. S6. UV-Visible absorption spectra showing host molecule **1** (5.8×10^{-6} M) in a CTAB micelle solution (9.0×10^{-3} M) assembled with dichloromethane (blue), and changes observed upon the addition of 20 molar equivalents of KPFOS (red).

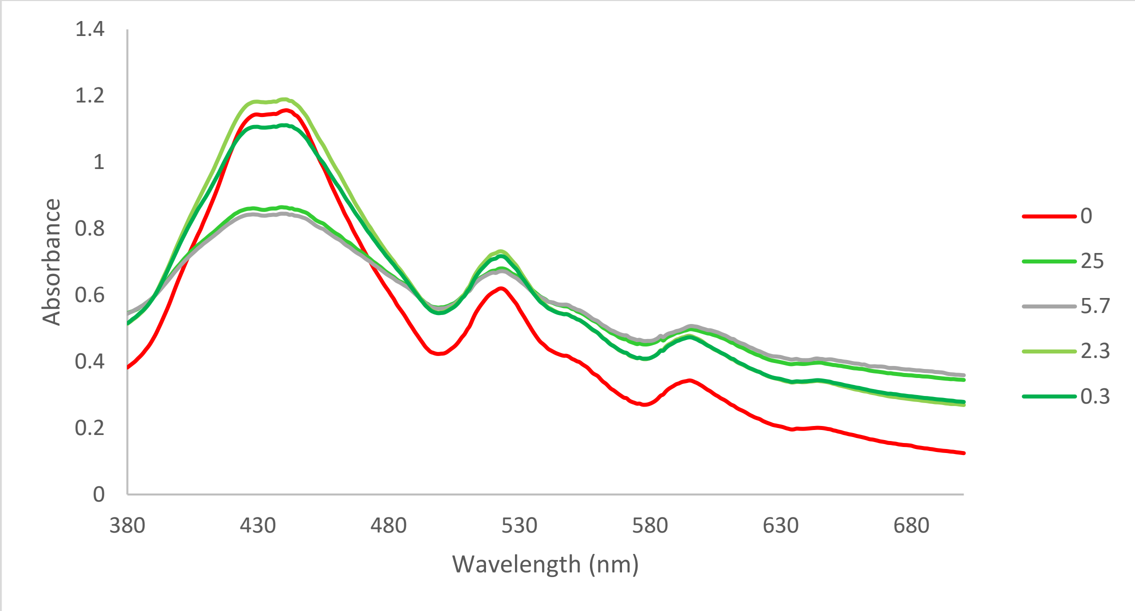

Fig. S7. UV-Visible absorption spectra showing the Soret band region of host molecule **1** (1.8×10^{-5} M) in an SDS micelle solution (7.3×10^{-3} M) assembled with acetone when combined with KPFOS (0, 0.3, 2.3, 5.7, and 25 ppm).

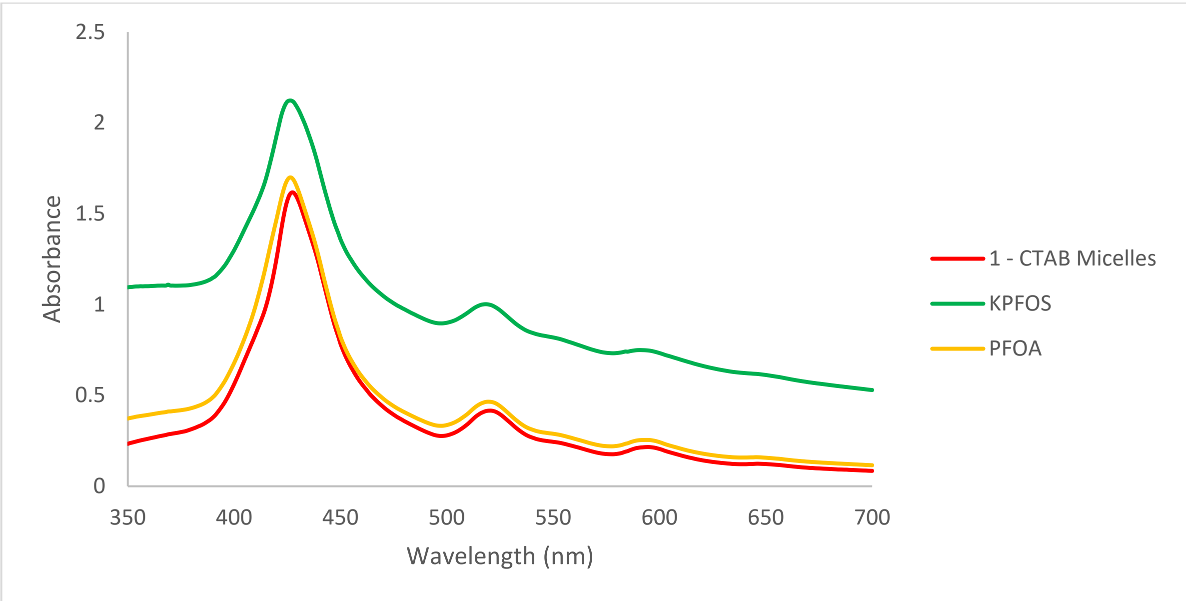

Fig. S8. UV-Visible absorption spectra showing host molecule **1** (2.2×10^{-5} M) in a CTAB micelle solution (9.0×10^{-3} M) assembled with THF (red), and changes observed upon the addition of 20 molar equivalents of KPFOS (green) and PFOA (yellow). The increased absorption is due to the scattering from precipitation.

RGB Analysis Methods

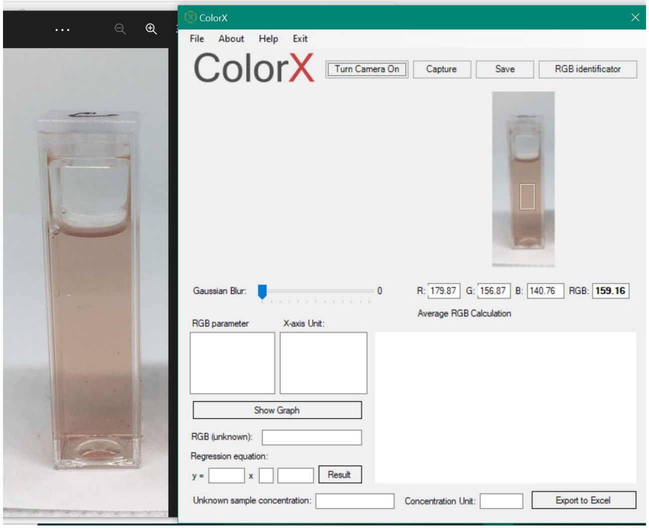

Fig. S9. Example of user-friendly RGB extraction from a mobile phone camera photograph using ColorX software.[1]

To quantify a color difference, RGB values are transformed within the CIELab color space using ImageJ. The difference, expressed as ΔE, is determined by measuring the relative distance between two colors.[2] The CIE76 algorithm transforms the L*a*b* coordinates according to the formula[3]:

$$\Delta E_{76} = \sqrt{(L^* - L^*_{Blank})^2 + (a^* - a^*_{Blank})^2 + (b^* - b^*_{Blank})^2}$$

The RGB parameter was determined according to the formula:

$$RGB\ Parameter = \frac{\Delta R + \Delta G + \Delta B}{R_H + G_H + B_H}$$

where: $\Delta R = |R_H - R_s|, \Delta G = |G_H - G_s|, \ \Delta B = |B_H - B_s|$

Here H indicates the values for the host solution, and S indicates the response for a sample containing PFAS so that ΔR, ΔG and ΔB give the color differences. The RGB parameter is the response due to the relative difference in the RGB intensities.

Host–Guest Concentrations

Table S2. Concentrations of host **1** and KPFOS in the final sample volumes.

Sample	**A**	**B**	**C**	**D**	
C(host)	5.31×10^{-6}	7.97×10^{-6}	1.06×10^{-5}	1.33×10^{-5}	[mol/L]
	12	18	24	30	ppm
C(KPFOS)	3.33×10^{-5}	2.50×10^{-5}	1.67×10^{-5}	8.33×10^{-6}	[mol/L]
	16	12	8	4	ppm
H:G Ratio	1:6	1:3	2:3	8:5	

Table S3. Concentrations of host **1** and KPFOS in the final sample volumes.

Sample	**A**	**B**	**C**	**D**	
C(host)	1.05×10^{-5}	1.05×10^{-5}	1.05×10^{-5}	1.05×10^{-5}	[mol/L]
	24	24	24	24	ppm
C(KPFOS)	1.25×10^{-5}	6.25×10^{-6}	3.13×10^{-6}	1.56×10^{-6}	[mol/L]
	6.2	3.1	1.6	0.8	ppm
H:G Ratio	4:5	5:3	23:7	47:7	

References

1. Šafranko S, Živković P, Stanković A, Medvidović-Kosanović M, Széchenyi A, Jokić S. Designing ColorX, image processing software for colorimetric determination of concentration, to facilitate students' investigation of analytical chemistry concepts using digital imaging technology. *J Chem Educ* 2019; 96(9): 1928-1937.
2. Hunt RWG, Pointer MR. *RGB Colorimetry. Measuring Colour*, 4th edn. Wiley; 2011. pp. 231-240.
3. Boronkay G. Colour Conversion Centre 4.0, http://ccc.orgfree.com/. 2021.